ATTEMPTS TO CALCULATE GLOBAL SOLUTIONS OF PROBLEMS THAT MAY HAVE LOCAL MINIMA

by

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INTRODUCTION

A particularly vexing problem in the solution of nonlinear optimization problems is the possibility that algorithms for solving the problem converge to local as opposed to global solutions. In this paper is contained an all too brief survey of proposals for obtaining global solutions to not necessarily convex optimization problems. In all cases an attempt will be made to point out the difficulties associated with the ideas.

CONVEX PROGRAMMING, CONVEX ENVELOPES AND THE GLOBAL SOLUTION

It is well known that a local solution to the problem

$$\min f(x) \quad \text{subject to} \quad g_i(x) \geq 0,\ i = 1,\ldots,m$$

where $x \in E^n$, $f(x)$, $\{-g_i(x)\}$, are donvex functions is also a global solution. An interesting proposal for solving for the global solution when the convexity assumptions do not hold has been proposed by Kleibohm [19]. The problem he addressed was slightly more general,

given as

min $f(x)$ subject to $x \epsilon B$ where f is continuous,

B a compact set.

Define CON(B) (the convex hull of B) as

$$CON(B) = \{x | x = \sum_{j=1}^{n} \lambda_j x_j, \ x_j \epsilon B\} \text{ where } \lambda_j \geq 0, \ \sum_{j=1}^{n} \lambda_j = 1 .$$

Define the largest convex subfunction $u(\cdot)$ as

1. $u(\cdot)$ is convex on CON(B)
2. $u(x) \geq f(x)$ for all $x \epsilon B$
3. $u(x) \geq q(x)$ for all $x \epsilon B$ for all functions $q(\cdot)$ having the propeties that
4. $q(\cdot)$ is convex on CON(B)
5. $q(x) \geq f(x)$ for all $x \epsilon B$.

He proves the following result.

The solution set of: min $u(x)$ subject to $x \epsilon CON(B)$ contains the solution set of: min $f(x)$ subject to $x \epsilon B$.

This interesting proposal has much theoretical interest and points out at least in an abstract geometrical manner how to solve the problem. The difficulties with it are threefold. The major problem is that it is impossible, except in certain special cases, to describe algebraically CON(B) and $u(\cdot)$. In more concrete terms, one cannot implement the algorithm on a digital computer. Second, it seems clear from some small examples that the function $u(\cdot)$ does not maintain the differentiability properties of the original function. Hence existing algorithms for solving a convex program could not be used. Finally, the solution to the convex programming problem need not be feasible to the original problem, although the solution values are the same.

THE USE OF GRIDS

One of the most obvious ways to solve a programming problem and one which is often suggested by those new to the field is the grid approach. The algorithm assumes lower and upper bounds on each variable, divides the resulting interval into I_j equally spaced intervals and finds the point over the grid with minimum objective function value which is feasible. The difficulty with this approach is the extraordinarily high number of function evaluations required for a problem with many variables. The number of possibilities, or combinations of points involved is $\prod_{j=1}^{n} I_j$. Many methods for obtaining global solutions essentially are of the grid type. The branch and bound technique for separable programming described later has elements of a grid search but is intended, like all branch and bound methods, to reduce the number of points considered by showing that subsets of the combinations cannot possibly contain the solution to the problem. Recent work by Hartley, et al., [14] falls into the category of a grid search method.

RANDOM METHODS

An idea akin to the grid approach for obtaining global solutions is the random method, and variations on this method. Basically the idea is to assume lower and upper bounds on the range of the variables and generate points within that range by a randomized procedure. Methods vary in the way the points are generated and how much use they make of previous information. A limited amount of experience by the author's student with the Russian approaches, Matyas [22], Motkus [25], showed evidence that the methods had a very slow rate of convergence and took an enormous number of function evaluations. Theoretically, of course, it is possible to show that the methods converge in the limit to the global solution with probability one.

THE LAGRANGIAN APPROACH

One often heralded approach to the programming problem is the use of the Lagrangian function $L(x,u) = f(x) - \Sigma u_i g_i(x)$ to obtain global solutions. Roughly stated, one generates a sequence of nonnegative multiplier vectors $\{u^k\}$ and an associated sequence $\{x^k\}$ of points which are the global unconstrained minimizers of the Lagrangian. If the values of $\{g_i(x^k)\}$ tend to zero for non-zero u_i^k limits, then limit points of $\{x^k\}$ are global solutions to the programming problem. The alleged ease of implementing this method for separable problems has made it attractive. Several points should be noted. First, in the case when there are no constraints the algorithm reduces to the tautology -- "to find the global unconstrained minimizer of $f(x)$, find the global unconstrained minimizer of $f(x)$," i.e., there is no algorithm in the sense of a prescribed iterative procedure for doing this. Second, in general for the nonconvex optimization problem, the Lagrange multipliers associated with the global solution and the solution point do not constitute a pair for which the Lagrangian has a global unconstrained minimizer at x^*. In a nonconvex problem the Lagrangian is usually nonconvex and has no unconstrained minimizer at all. In the convex problem the difficulty with the Lagrangian approach is just to find the proper multipliers. In [5] Falk has shown the conditions under which such an algorithm would work for the convex case.

In another paper, Falk [6] characterized the solution obtained by the Lagrangian approach to the problem min $f(x)$ subject to $x \geq b$, $x \in G$, where G is a compact convex set as the solution to the minimization of $c(x)$ subject to $Ax \geq b$, $x \in G$ where $c(x)$ is the convex enveloped of $f(x)$ over G. (Recall from the theorem of Kleibohm the minimization should be of the convex envelope of $f(x)$ over $\{G \cap Ax \geq b\}$ to obtain the same solution). For more complicated problems the solution obtained is not easy to characterize but it is certainly not the correct one.

Example 1

To make the point more explicitly, consider the problem

$$\text{minimize } - x_1^2 - x_2^2$$

$$\text{subject to } - x_1 - 4x_2 + 5 \geq 0,\ - x_1 + 1 \geq 0,\ x_1 \geq 0,\ x_2 \geq 0 .$$

This problem has two local minimizers. Form the Lagrangian function

$$L(x,u) = - x_1^2 - x_2^2 - u_1(- x_1 - 4x_2 + 5) - u_2(- x_1+1) - u_3(x_1) - u_4(x_2) .$$

Now for no choice of multipliers does this Lagrangian function have a finite unconstrained minimizer.

The second order necessary conditions characterizing a local minimizer to a nonconvex programming problem indicate very clearly that the Lagrangian is in some sense minimized (again, speaking roughly) at x^* only in directions orthogonal to the gradients of the binding constraints. Hence, basing a method on finding the unconstrained minimizer of the Lagrangian is doomed to fail since it does not take into account the fundamental characteristics which apply to a local (and hence global) minimizer to a nonlinear programming problem.

THE PENALTY FUNCTION APPROACH

An easy theorem to prove is that if one applies an interior point unconstrained penalty function to a nonconvex programming problem, such as that given by (1) and (2), e.g., if one obtains the global minimizer x^k of $f(x) - r_k \Sigma \ell n g_i(x)$ for a decreasing sequence of values $\{r_k\}$ which tend to zero, then the global unconstrained minimizers approach the global unconstrained solution $(x^k \to x^*)$ in the limit as $r_k \to 0$. Unlike the Lagrangian approach, the existence of the global unconstrained minimizer in the interior of the feasible region usually obtains in the nonconvex situation. For example, if $\{x | f(x) \leq M,\ g_i(x) \geq 0,\ i = 1, \ldots, m\}$ is

bounded for all M (which it usually is in practice), then a global minimizer of the penalty function exists. The difficulty here is that there is no guarantee that one can obtain a global -- as opposed to local -- unconstrained minimizer. In fact, one can show that a sequence of unconstrained local minimizers exists which approach every isolated compact set of local constrained minimizers. In the problem of Example 1, using a penalty function approach would yield either of the local minimizers depending upon the initial starting point. The penalty function approach is then, not primarily intended to be a global method in the nonconvex case.

(It should be noted that the existence of a global unconstrained minimizer for exterior point penalty functions does not follow under the same circumstances and may generate unbounded sequences of points.)

METHODS OF SUCCESSIVE FEASIBILITY

Many investigators have produced algorithms for obtaining global solutions which are variations of the general idea of the elimination of local minimizers once they are obtained by the addition of constraints which eliminate the local minimizer. Such an idea where spheres around the local minimizer are introduced is contained in Hesse [15]. As a heuristic such ideas might have merit, but in general there is a great deal of parameter selection necessary (such articles are full of experimentation with $\varepsilon = .1, .001\ldots$), and as a theoretical device are fraught with difficulties. Two objections are immediate. In some cases the new constraints introduced generate programming problems where the local minimizers are not local minimizers of the original problem. In others such as min $f(x)$ subject to

$$g_i(x) \geq 0, \quad i = 1,\ldots,m, \ f(x) \leq f(x^k) - \varepsilon$$

where x^k is a local minimizer previously found, the question is [illegible] since in a neighborhood of x^k there is no point feasible

to the problem. The problem of finding a feasible point is itself an optimization problem and is subject to the same difficulties as the original one.

NONCONVEX QUADRATIC PROGRAMMING

The area of finding global solutions to not necessarily convex quadratic programming problems has an extensive literature and will not be discussed here. The first major paper was published by Ritter [30]. Recent work of Cottle and Mylander [3] explains and expands this work. When the quadratic form (to be minimized) is negative semi-definite, the global (and any local solution) is at a vertex. Using this fact several authors have made suggestions on how best to find it -- Tui [35], Hu [17], Cabot and Francis [2].

Other work on the quadratic indefinite form has been done by Mueller and Cooper [26].

GEOMETRIC PROGRAMMING AND DIFFERENTIABLY UNIMODAL FUNCTIONS

The class of functions for which local minimization implies global minimization is not restricted to those where the functions are convex. A very general class for which this is true is (see Mangasarian [21])

minimize $f(x)$ (a pseudo convex function)

subject to $g_i(x) \geq 0$, $i = 1,\ldots,m$ where each g_i is a quasi concave function). It is well-known also that Geometric Programming Problems have the local global property even though the functions involved are not pseudo-convex or quasi-concave. In a recent paper, Zwart [39] showed for a class of functions with certain properties, local solutions are global solutions. His classification covered the case of geometric programming. The main development is repeated here. A function f is a differentially unimodal function on an open set R if f is

differentiable on R and if when for some point $\bar{x}\epsilon R$ $\nabla f(\bar{x}) = 0$ holds it is implied that $\bar{x}$ is a global minimizer for f restricted to R. (Such a point need not exist.)

<u>Theorem</u> (Zwart [39], p. 157)

Suppose that F is a family of functions for which (i) $f\epsilon F \rightarrow f$ is differentiably unimodal on R, (ii) $f\epsilon F \rightarrow \alpha f\epsilon F$ for any positive real number α, and (iii) $f_1\epsilon F$, $f_2\epsilon F \rightarrow f_1 + f_2\epsilon F$. Then any problem of the form

$$\text{minimize} \quad f(x) \quad \text{subject to} \quad g_i(x) \geq 0, \; i = 1,\ldots,m$$

where f, $\{-g_i\}\epsilon F$, $i = 1,\ldots,m$ must have the property that any local minimizer is a global minimizer.

Analyses such as that above may serve to bring the special characteristics of geometric programming into a synthesis with the properties of convex programming. Currently work on obtaining global solutions to geometric programming problems when the signs on the posynomial coefficients are improper is under way -- see Duffin and Peterson [4] and the references therein.

MISCELLANEOUS METHODS

Some interesting results on a theoretical level which may lead to procedures for obtaining global minimizers have been suggested in several places. There is no way to categorize these except possibly to say that they all involve using the integrals of the objective function rather than the derivatives. Abbreviated summaries of these results follow.

<u>Theorem</u> (Falk [7])

Suppose the programming problem is

$$\max \quad f(x) \quad \text{(continuous)}$$

subject to $x\epsilon S$ the closure of a bounded domain where without loss of generality it can be assumed that $f(x) \geq \alpha > 0$ for all $x\epsilon S$. Then a point $x^*\epsilon S$ is <u>not</u> a global minimizing point for this problem if, for some $n > 0$,

$$\int_S [f(x)/f(x^*)]^{n+1} > \int_S [f(x)/f(x^*)]^n$$

<u>**Theorem**</u> **(Falk [7])**

A necessary and sufficient condition that a point x^* solve the problem above is that

$$\limsup_{t \to \infty} \int_S [f(x)/f(x^*)]^t < \infty .$$

An explicit representation of the point which is the global solution of the above problem was given by Pincus [28].

Assume that for the above problem, f attains its global minimum at exactly one point x^*. Then the co-ordinates of the minimizing point are given as

$$x_j^* = \lim_{\lambda \to \infty} \frac{\int_S x_j e^{\lambda f(x)}}{\int_S e^{\lambda f(x)}} ,$$

THE BRANCH AND BOUND APPROACH

Almost all optimization problems which can be implemented on a digital computer are capable of being converted into equivalent separable programming problems by the addition of variables and equality constraints. A method for solving a nonlinear optimization problem with convex constraints using the branch and bound approach was suggested by Falk and Soland [8] when the objective function was separable in the nonconvex portion. Later the algorithm was extended by Soland [33] to handle separable nonconvex constraints.

Computer implementation of the idea, which relies heavily on the concept of convex envelopes, has been highly successful in

certain cases, particularly when the subproblems generated by the branch and bound algorithm could be handled by linear programming subroutines. A brief description of the algorithm is as follows.

The problem addressed is

$$\text{minimize} \quad f(x) = \Sigma_{j=1}^{n} f_j(x_j)$$

subject to

$$x \varepsilon G \quad \text{(a closed set)} ,$$

$$x \varepsilon C \equiv \{x | \ell \leq x \leq L\} ,$$

$$g_i(x) = \Sigma_{j=1}^{n} g_{ij}(x_j) \leq 0, \; i = 1,\ldots,m .$$

For each j, f_j and all g_{ij} must be lower semi-continuous on the finite interval $[\ell_j, L_j]$. It is further assumed that the set of points $G \cap H$ is nonempty where H is defined as

$$H \equiv \{x | x \varepsilon C, g_i(x) \leq 0, \; i = 0,\ldots,m\} .$$

These assumptions are enough to ensure that f attains its minimum over the set $G \cap H$.

The algorithm produces a sequence of (not necessarily feasible) points $\{x^k\}$. Each x^k is a solution of problem P^{kv_k} which involves the minimization of a convex function over the intersection of G with a convex set contained in C. Branching is the partitioning of C into smaller and smaller rectangles, and the lower bounds are lower bounds of f over the intersection of each of these rectangles with $G \cap H$.

Crucial to the algorithm is the use of convex envelopes to provide underestimating convex functions of the original problem functions. Let $C^{kv} = \{x | \ell^{kv} \leq x \leq L^{kv}\}$. In problem P^{kv} f_j is replaced by its convex envelope ψ_j^{kv} over $[\ell_j^{kv}, L_j^{kv}]$, and each g_{ij} by its convex envelope Θ_{ij}^{kv} over $[\ell_j^{kv}, L_j^{kv}]$.

Let

$$\psi^{kv}(x) \equiv \Sigma_{j=1}^{n} \ \psi_j^{kv}(x_j) \ ,$$

$$\theta_i^{kv}(x) \equiv \Sigma_{j=1}^{n} \ \theta_{ij}^{kv}(x), \quad i = 1,\dots,m$$

so that ψ^{kv} is the convex envelope of f over C^{kv} and θ_i^{kv} is the convex envelope of g_i over C^{kv} .

As a computational aside, it is very simple to compute the convex envelope of a simple function of a single variable over an interval in most practical cases. For example, if the function is concave, its convex envelope is a straight line. The process can be implemented on a computer so that this is an automatic procedure for standard functions as $\sin(x)$, $-e^x$, $x^{.1}$.

The programming problem P^{kv} associated with any rectangle C^{kv} is then

$$\text{minimize} \quad \psi^{kv}$$

subject to

$$x \in G,$$
$$x \in C^{kv} \equiv \{x \mid \ell^{kv} \le x \le L^{kv}\} \ ,$$
$$\theta_i^{kv}(x) \le 0, \ i = 1,\dots,m \ .$$

By construction it is easy to show that x^{kv}, any solution point to P^{kv} is a lower bound to f over $G \cap H \cap C^{kv}$.

At any stage k the original rectangle C has been subdivided into p_k rectangles which together constitute a partition $P^k = \{C^{k1},\dots, C^{kp_k}\}$. Associated with each rectangle C^{kv} are convex underestimating envelopes $\{\psi^{kv}\}$, $\{\theta_i^{kv}\}$, and a programming problem P^{kv} with solution point x^{kv}. Attention is focused on the rectangle whose objective function value is smallest. That is, let v_k denote an integer

where
$$\psi^{kv_k}(x^{kv_k}) = \min_v \psi^{kv}(x^{kv}), \ v = 1,\ldots,p_k .$$
For simplicity, let x^k denote x^{kv_k}. The termination rule for the algorithm is that if $f(x^k) = \psi^{kv_k}(x^k)$, and if $x^k \varepsilon H$, then the problem is solved by x^k. This is true because
$$\psi^{kv_k}(x^k) \le \psi^{kv}(x) \le f(x)$$
for all $x \varepsilon G \cap H \cap C^{kv}$ and $v = 1,\ldots,p_k$. If $f(x^k) > \psi^{kv_k}(x^k)$ and/or $x^k \notin H$ the algorithm proceeds to stage $k + 1$ by dividing the rectangle C^{kv_k} into two or more rectangular subsets.

The branching part of the algorithm takes two forms depending on whether or not the problem functions are continuous or merely lower-semicontinuous.

Weak Branching Rule

Choose any j that maximizes the difference
$$f_j(x_j^k) - \psi_j^{kv_k}(x_j^k)$$
or
$$g_{ij}(x_j^k) - \Theta_{ij}^{kv_k}(x_j^k)$$

where i is restricted to the infeasible constraints, i.e., those for which $g_i(x^k) > 0$. Then $p_{k+1} = p_k + 1$, i.e., two new rectangles are formed by splitting C^{kv_k} into two parts. The bounds for both new rectangles are the same for all components except the jth which in one case has $[\ell_j^{kv_k}, x_j^k]$ as its bounds, and in the other, $[x_j^k, L_j^{kv_k}]$.

Strong Branching Rule

For <u>every</u> j such that

$$f_j(x_j^k) - \psi_j^{kv_k}(x_j^k) > 0$$

or

$$g_{ij}(x_j^k) - \theta_{ij}^{kv_k}(x_j^k) > 0$$

for those i such that $g_i(x^k) > 0$, divide the corresponding interval $[\ell_j^{kv_k}, L_j^{kv_k}]$ into the two intervals $[\ell_j^{kv_k}, x_j^k]$ and $[x_j^k, L_j^{kv_k}]$, creating a new rectangle for stage $(k+1)$ for every such j.

Note that the strong branching rule in general generates many more new rectangles (and hence programming problems to be solved) than the weak branching rule. Its use is to be avoided if possible. However, it may be needed to guarantee convergence of the algorithm. Two statements about convergence are stated in the following theorems.

<u>Theorem</u> -- If the strong branching rule is used to generate new rectangles, then any limit point of $\{x^k\}$ is a solution of problem P.

<u>Theorem</u> -- If the functions $f, \{g_i\}$ are continuous, and if the weak branching rule is used to generate the new rectangles, then every limit point of $\{x^k\}$ is a solution of problem P.

More details, and illustrative examples are contained in Falk and Soland [8], and Soland [35]. A similar approach to the problem using concepts of <u>special ordered sets</u> has been proposed by Beale and Tomlin [1], and Tomlin [34]. Their piece-wise-linear approximation approach allows the use of linear programming codes to solve the sequences of subproblems generated by this branch and bound method.

A general approach which uses the integral of the function over the feasible domain has been proposed by Graves and Whinston [13]. This proposal has elements of the grid approach but with a refinement procedure for creating smaller rectangles similar to that of Falk and Soland discussed in the previous section. Instead of choosing the rectangle with the smallest lower bound for branching, they compute the average value of the function over the region and subdivide the rectangle with smallest average value. As the area of the nested rectangle goes to zero, the average value approaches the value of the limiting point. (This is an abbreviated description of their more general approach.) They have successfully solved some small problems. Difficulties in using this method stem computationally from the problem of computing the average value (they give several approximation schemes for this) and the lack of a valid convergence criterion other than an exhaustive subdivision of all the rectangles.

SUMMARY

Almost all of the algorithms suggested for obtaining global solutions to nonconvex programming problems contain some aspect which make their implementation impossible, or elements which required a combinatorially unacceptable amount of computer work. The branch and bound approach, relying on use of underestimating convex functions seems the most reasonable approach at this time. The efficiency it offers depends upon how quickly the regions which do not contain the global solution are eliminated.

In many instances the solution to a nonconvex problem obtained by an algorithm which obtains local minimizers can be seen to be the solution. The branch and bound method takes no advantage of the fact a good guess at the solution is available. Rather than as an algorithm for solving the problem, one should probably regard the branch and bound algorithm as a verification procedure. Then its use, which is invariably longer in computer time than an algorithm which directly tries to obtain local solutions can be made greater or lesser by those who formulate the problem to be solved.

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